

CHAPTER 6

MASTER EQUATION AND REACTION-DIFFUSION EQUATION

[This chapter is based on the lectures of Professor Hans J. Haubold of the Office of Outer Space Affairs, United Nations, Vienna, Austria at the 2008 SERC School.]

6.0. Introduction

Time variation and pattern formation in complex and dynamical systems is an active research area in non-equilibrium statistical physics. Mathematical modeling of such systems and inferring the underlying deterministic and stochastic processes from time series is based on master equations. Reaction-diffusion equations are derived from master equations, taking into account certain physical and mathematical conditions. Reaction equations (kinetic equations) for jump processes and diffusion equations for random walks are the simplest versions of master equations. Such equations, and their fractional generalizations, are used to describe stochastic processes in non-equilibrium physical systems. A common assumption for them is the Markov property and thus the processes under consideration have no memory. Special utility for master equations is the principle of detailed balance as is for reaction-diffusion equations the mass action law. A stochastic process is represented by the time evolution of a random variable. If Y is a random variable, the stochastic process is $Y(t)$. A stochastic variable is defined by specifying the set of possible values called set of states (space of events, phase space) and by a probability distribution over this set. The set can be discrete (e.g. number of species of a component in a reaction) or continuous (e.g. the velocity of a Brownian particle). A classical field where stochastic processes are essential is statistical mechanics. Statistical mechanics studies systems of large numbers of species. Average values characterizing such species are measured through probability considerations. The concept of statistical mechanics is replacing the system by an ensemble of realizations, i.e. a collection of microstates of the system under consideration. This ensemble serves to visualize the probability distribution over the set of microstates. A classical example of a stochastic process is Brownian motion, i.e. the motion of a heavy colloidal particle immersed in a fluid made up of light particles. The stochastic variable $Y(t)$ in this case can be the position or velocity of the Brownian particle. If $Y(t)$ were deterministic, one could find an expression for the evolution of Y in time, such as to give Y at each t . Because Y is a stochastic variable, each instant of t does not have a specific value for Y , but a probability for the value of Y .

6.1. Markov Processes

In order to understand the Markov property, the conditional probability is being defined. The conditional probability $P_{1|1}(y_2, t_2|y_1, t_1)$ is defined through the following relation

$$P_2(y_1, t_1; y_2, t_2) = P_{1|1}(y_2, t_2|y_1, t_1)P_1(y_1, t_1) \quad (6.1.1)$$

which means that the joint probability of finding y_1 at t_1 and y_2 at t_2 equals the probability of finding y_1 at t_1 times the probability of finding y_2 at t_2 , given y_1 at t_1 . The conditional probability satisfies the following properties

1. $P_{1|1} \geq 0$
2. $\int P_{1|1}(y_2, t_2|y_1, t_1)dy_2 = 1$
3. $P_1(y_2, t_2) = \int P_{1|1}(y_2, t_2|y_1, t_1)P_1(y_1, t_1)dy_1.$

Property 3 follows from equation (6.1.1), when integrated over y_1 . Integrating the left-hand side of (6.1.1) over y_1 gives $P_2(y_1, t_1; y_2, t_2)dy_1 = P_1(y_2, t_2)$, i.e. $P_1(y_2, t_2)$ is the marginal probability distribution of P_2 with respect to y_2 .

A Markov process is defined by the following relation, which is called Markov property

$$P_{1|n-1}(y_n, t_n|y_{n-1}, t_{n-1}; \dots; y_1, t_1) = P_{1|1}(y_n, t_n|y_{n-1}, t_{n-1}), \quad t_1 < t_2 < \dots < t_n. \quad (6.1.2)$$

The Markov property expresses that, for a Markov process, the probability of a transition at time t_{n-1} from a value y_{n-1} to a value y_n at time t_n depends only on the value of y at the time t_{n-1} , and not on the previous history of the system. Markov processes do not have memory. $P_{1|1}$ is called the transition probability.

For a Markov process the joint probabilities for $n \geq 3$ are all expressed in terms of P_1 and $P_{1|1}$. For $n = 3$

$$\begin{aligned} P_3(y_1, t_1; y_2, t_2; y_3, t_3) &= P_2(y_1, t_1; y_2, t_2)P_{1|2}(y_3, t_3|y_1, t_1; y_2, t_2) \\ &= P_1(y_1, t_1)P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2). \end{aligned} \quad (6.1.3)$$

Chapman-Kolmogorov equation

Considering equation (6.1.3), integrating it over y_2 and dividing both sides by P_1 gives the Chapman-Kolmogorov equation

$$P_{1|1}(y_3, t_3|y_1, t_1) = \int P_{1|1}(y_3, t_3|y_2, t_2)P_{1|1}(y_2, t_2|y_1, t_1)dy_2 \quad (6.1.4)$$

This equation states that a process starting at t_1 with value y_1 reaches y_3 at t_3 via any one of the possible values y_2 at the intermediate time t_2 .

Proof of (6.1.4)

$$\begin{aligned}
P_3(y_1, t_1; y_2, t_2; y_3, t_3) &= P_1(y_1, t_1)P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2) \\
\int P_3(y_1, t_1; y_2, t_2; y_3, t_3)dy_2 &= \int P_1(y_1, t_1)P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2)dy_2 \\
P_2(y_1, t_1; y_3, t_3) &= P_1(y_1, t_1) \int P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2)dy_2 \\
P_{1|1}(y_3, t_3|y_1, t_1)P_1(y_1, t_1) &= P_1(y_1, t_1) \int P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2)dy_2 \\
P_{1|1}(y_3, t_3|y_1, t_1) &= \int P_{1|1}(y_2, t_2|y_1, t_1)P_{1|1}(y_3, t_3|y_2, t_2)dy_2.
\end{aligned}$$

Definition of two types of Markov processes

Stationary: A process Y is stationary if it is not affected by a shift in time, i.e. $Y(t)$ and $Y(t + \epsilon)$ have the same probability distribution.

Homogeneous: A homogeneous process is a non-stationary Markov process defined by the probability $P^*(y_1) \equiv P_{1|1}(y_1|y_0)$. For such processes the transition probability depends only on the time interval $\tau = t_2 - t_1$.

For both stationary and homogeneous processes, a special notation is used for the transition probability and the Chapman-Kolmogorov equation

$$P_{1|1}(y_2, t_2|y_1, t_1) = T_\tau(y_2|y_1) \quad (6.1.5)$$

$$T_{\tau+\tau'}(y_3|y_1) = \int T_{\tau'}(y_3|y_2)T_\tau(y_2|y_1)dy_2. \quad (6.1.6)$$

Master equation

Taking the transition probability $T_{\tau'}$ and expanding it in a Taylor series over zero, considering small τ' , gives

$$T_{\tau'}(y_3|y_2) = \delta(y_2 - y_3) + \tau'W(y_3|y_2) + \mathcal{O}(\tau'^2) \quad (6.1.7)$$

The delta function expresses that the probability to stay at the same state after time zero equals one, whereas the probability to change state after time zero equals zero. $W(y_3|y_2)$ is the time derivative of the transition probability at $\tau' = 0$. Thus it is called transition probability per unit time.

This expression must satisfy the normalization property. Therefore the integral over y_3 must equal one. In order for that to happen, the above form must be corrected in the following sense

$$T_{\tau'}(y_3|y_2) = (1 - \alpha_0\tau')\delta(y_2 - y_3) + \tau'W(y_3|y_2) + \mathcal{O}(\tau'^2) \quad (6.1.8)$$

where the delta function has been corrected by the coefficient $1 - \alpha_0\tau'$ which corresponds to the probability for no transition to have taken place at all. Therefore

$$\alpha_0(y_2) = \int W(y_3|y_2)dy_3. \quad (6.1.9)$$

Putting equation (6.1.8) into equation (6.1.6), dividing by τ' and going to the limit $\tau' \rightarrow 0$ gives the differential form of the Chapman-Kolmogorov equation which is named master equation

$$\frac{\partial}{\partial \tau} T_{\tau}(y_3|y_1) = \int [W(y_3|y_2)T_{\tau}(y_2|y_1) - W(y_2|y_3)T_{\tau}(y_3|y_1)]dy_2. \quad (6.1.10)$$

Proof of (6.1.10)

Putting equation (6.1.8) in equation (6.1.6) gives

$$\begin{aligned} T_{\tau+\tau'}(y_3|y_1) &= \int T_{\tau'}(y_3|y_2)T_{\tau}(y_2|y_1)dy_2 \\ &= \int [(1 - \alpha_0\tau')\delta(y_2 - y_3) + \\ &\quad \tau'W(y_3|y_2)]T_{\tau}(y_2|y_1)dy_2 \\ &= \int T_{\tau}(y_2|y_1)\delta(y_2 - y_3)dy_2 - \\ &\quad \tau' \int \alpha_0(y_2)\delta(y_2 - y_3)T_{\tau}(y_2|y_1)dy_2 + \\ &\quad \tau' \int W(y_3|y_2)T_{\tau}(y_2|y_1)dy_2 \\ &= T_{\tau}(y_3|y_1) - \tau' \int W(y_2|y_3)T_{\tau}(y_3|y_1)dy_2 + \\ &\quad \tau' \int W(y_3|y_2)T_{\tau}(y_2|y_1)dy_2 \\ \frac{T_{\tau+\tau'}(y_3|y_1) - T_{\tau}(y_3|y_1)}{\tau'} &= \int [W(y_3|y_2)T_{\tau}(y_2|y_1) - W(y_2|y_3)T_{\tau}(y_3|y_1)]dy_2 \\ \frac{\partial T_{\tau}(y_3|y_1)}{\partial \tau} &= \int [W(y_3|y_2)T_{\tau}(y_2|y_1) - W(y_2|y_3)T_{\tau}(y_3|y_1)]dy_2 \end{aligned}$$

Noting that all transition probabilities are for a given value y_1 at t_1 , one may write, suppressing indices

$$\frac{\partial P(y, t)}{\partial t} = \int [W(y|y')P(y', t) - W(y'|y)P(y, t)]dy'. \quad (6.1.11)$$

This is the master equation for a jump process. If the range of Y is a discrete set of states with labels n , the equation reduces to

$$\frac{dp_n(t)}{dt} = \sum_{n'} [W_{nn'}p'_{n'}(t) - W_{n'n}p_n(t)]. \quad (6.1.12)$$

In terms of physics, the master equation is a gain-loss equation for the probability of each state n . The first term is the gain due to transitions from other states n , and the second term is the loss due to transitions into other states n .

Under steady state condition, the left side of the master equation equals zero. Therefore the steady state condition property has the form

$$\sum_{n'} W_{nn'}p'_{n'} = \left(\sum_{n'} W_{n'n} \right) p_n. \quad (6.1.13)$$

This relation expresses the fact that in steady state, the sum of all transitions per unit time into any state n must be balanced by the sum of all transitions from n

into other states n' . Detailed balance is the stronger assertion that for each pair n, n' separately the transitions must balance

$$W_{nn'}P'_n = W_{n'n}P_n. \quad (6.1.14)$$

Detailed balance is a necessary but not sufficient condition for thermodynamic equilibrium. In terms of quantum mechanics, detailed balance in thermodynamic equilibrium follows from microscopic reversibility. However, it may also hold in some cases for non-equilibrium. Therefore, thermodynamic equilibrium is the strongest condition (sufficient but not necessary).

Mean-field equation

Let Y be a physical quantity with Markov character. The master equation determines its probability distribution at all $t > 0$. In ordinary macroscopic physics, however, one ignores fluctuations and treats Y as if it were a non-stochastic, single-valued quantity $\langle Y \rangle$. The evolution of $\langle Y \rangle$ is described by a deterministic differential equation for $\langle Y \rangle$ called the mean-field equation. As the master equation determines the entire probability distribution, it must be possible to derive from it the mean-field equation as an approximation for the case that fluctuations are negligible.

The following exact identity holds

$$\begin{aligned} \frac{d}{dt} \langle Y \rangle (t) &= \int y \frac{\partial P(y, t)}{\partial t} dy \\ &= \int \int [W(y|y')P(y', t) - W(y'|y)P(y, t)] dy dy' \\ &= \int \int (y' - y)W(y'|y)P(y, t) dy dy' \\ &= \int a_1(y)P(y, t) dy = \langle a_1(y) \rangle. \end{aligned} \quad (6.1.15)$$

Proof of (6.1.15)

$$\begin{aligned} \frac{d}{dt} \langle Y \rangle (t) &= \int \int y [W(y|y')P(y', t) - W(y'|y)P(y, t)] dy dy' \\ &= \int \int y W(y|y')P(y', t) dy dy' - \int \int y W(y'|y)P(y, t) dy dy' \\ &= \int \int y' W(y'|y)P(y, t) dy dy' - \int \int y W(y'|y)P(y, t) dy dy' \\ &= \int \int (y' - y)W(y'|y)P(y, t) dy dy' \\ &= \int a_1(y)P(y, t) dy = \langle a_1(y) \rangle. \end{aligned}$$

The jump moments $a_\nu(y)$ are defined by

$$a_\nu(y) = \int (y' - y)^\nu W(y'|y) dy', \quad \nu = 0, 1, 2, \dots \quad (6.1.16)$$

Therefore, the mean-field equation for the time evolution $\langle Y \rangle(t)$, if $a_1(y)$ is a linear function of y , is given by

$$\frac{d}{dt} \langle Y \rangle = a_1(\langle Y \rangle). \quad (6.1.17)$$

If, however, $a_1(\langle Y \rangle)$ is not a linear function of $\langle Y \rangle$, one has a different form for $a_1(\langle Y \rangle)$ by expanding it into a Taylor series over $\langle Y \rangle$.

$$\langle a_1(Y) \rangle = a_1(\langle Y \rangle) + \frac{1}{2} \langle (Y - \langle Y \rangle)^2 \rangle a_1''(\langle Y \rangle) + \dots \quad (6.1.18)$$

Proof of (6.1.19)

Taylor series of $a_1(Y)$ over $\langle Y \rangle$

$$a_1(Y) = a_1(\langle Y \rangle) + a_1'(\langle Y \rangle)(Y - \langle Y \rangle) + \frac{1}{2} a_1''(\langle Y \rangle)(Y - \langle Y \rangle)^2 + \dots$$

The mean value of the above is

$$\begin{aligned} \langle a_1(Y) \rangle &= a_1(\langle Y \rangle) + a_1'(\langle Y \rangle) \langle (Y - \langle Y \rangle) \rangle + \\ &\quad \frac{1}{2} a_1''(\langle Y \rangle) \langle (Y - \langle Y \rangle)^2 \rangle + \dots \end{aligned}$$

Considering that

$$\langle (Y - \langle Y \rangle) \rangle = 0 : \langle a_1(Y) \rangle = a_1(\langle Y \rangle) + \frac{1}{2} \sigma^2 a_1''(\langle Y \rangle).$$

The evolution of $\langle Y \rangle$ in the course of time is therefore not determined by $\langle Y \rangle$ itself, but is influenced by the fluctuations around this average (variance σ^2). Thus for nonlinear $a_1(\langle Y \rangle)$ we need an equation for the variance as well.

Similar to what was done for $\langle Y \rangle$

$$\begin{aligned} \frac{d}{dt} \langle Y^2 \rangle &= \int \int (y'^2 - y^2) W(y'|y) P(y) dy dy' \\ &= \int \int [(y' - y)^2 + 2y(y' - y)] W(y'|y) P(y) dy dy' \\ &= \langle a_2(Y) \rangle + 2 \langle Y a_1(Y) \rangle. \end{aligned}$$

This is identical with

$$\frac{d\sigma^2}{dt} = \langle a_2(Y) \rangle + 2 \langle (Y - \langle Y \rangle) a_1(Y) \rangle \quad (6.1.19)$$

Proof of (6.1.19)

$$\begin{aligned}
\frac{d}{dt} \langle Y^2 \rangle &= \int y^2 \frac{dP(y)}{dt} dy \\
&= \int \int y^2 [W(y|y')P(y') - W(y'|y)P(y)] dy dy' \\
&= \int \int y^2 W(y|y')P(y') dy dy' - \int \int y^2 W(y'|y)P(y) dy dy' \\
&= \int \int y'^2 W(y'|y)P(y) dy dy' - \int \int y^2 W(y'|y)P(y) dy dy' \\
&= \int \int (y'^2 - y^2) W(y'|y)P(y) dy dy' \\
&= \int \int [(y' - y)^2 + 2y(y' - y)] W(y'|y)P(y) dy dy' \\
&= \langle a_2(Y) \rangle + 2 \langle Y a_1(Y) \rangle .
\end{aligned}$$

One has

$$\begin{aligned}
\frac{d\sigma^2(t)}{dt} &= \frac{d \langle Y^2 \rangle}{dt} - \frac{d \langle Y \rangle}{dt} \langle Y \rangle \\
&= \frac{d \langle Y^2 \rangle}{dt} - 2 \frac{d \langle Y \rangle}{dt} \langle Y \rangle \\
&= \langle a_2(Y) \rangle + 2 \langle Y a_1(Y) \rangle - 2 \langle Y \rangle \langle a_1(Y) \rangle \\
&= \langle a_2(Y) \rangle + 2 \langle (Y - \langle Y \rangle) a_1(Y) \rangle \\
&= \langle a_2(Y) \rangle + 2 \langle (Y - \langle Y \rangle) a_1(\langle Y \rangle) \rangle + \\
&\quad a'_1(\langle Y \rangle) (Y - \langle Y \rangle)^2 + \dots \rangle \\
&= \langle a_2(Y) \rangle + 2 \langle Y - \langle Y \rangle \rangle a_1(\langle Y \rangle) + \\
&\quad 2 a'_1(\langle Y \rangle) \langle (Y - \langle Y \rangle)^2 \rangle \\
&= a_2(\langle Y \rangle) + 2 \sigma^2 a'_1(\langle Y \rangle).
\end{aligned}$$

Replacing $\langle Y \rangle (t)$ with $y(t)$ we get the two equations that constitute the first approximation beyond the mean-field equation

$$\dot{y} = a_1(y) + \frac{1}{2} \sigma^2 a''_1(y) \quad (6.1.20)$$

$$(\dot{\sigma}^2) = a_2(y) + 2 \sigma^2 a'_1(y). \quad (6.1.21)$$

One-step processes

There is an important family of Markov processes, called production-destruction processes or birth-death processes, which are called one-step processes. These processes are continuous in time, their range consists of integers n , and only jumps between adjacent states are permitted. The master equation for such processes is

$$\dot{p}_n = r_{n+1} p_{n+1} + g_{n-1} p_{n-1} - (r_n + g_n) p_n \quad (6.1.22)$$

where r_n is the probability per unit time for a jump from state n to state $n - 1$ and g_n is the probability per unit time for a jump from n to $n + 1$. One-step processes can be subdivided based on the coefficients r_n and g_n into the following categories

- Linear, if the coefficients are linear functions of n
- Nonlinear, if the coefficients are nonlinear functions of n
- Random walks, if the coefficients are constant

One example of a random walk is the Poisson process. The Poisson process calculates the probability of n events occurring at time $t > 0$. The Poisson process is defined by

$$r_n = 0, \quad g_n = q, \quad p_n(0) = \delta_{n,0} \quad (6.1.23)$$

No destruction exists and q is a constant. The Kronecker delta expresses that the probability for no events to have occurred after time zero equals one, and the probability of more than one event occurring after time zero equals zero. The master equation for the Poisson process has the form

$$\dot{p}_n = q(p_{n-1} - p_n) \quad (6.1.24)$$

which has the following solution

$$p_n(t) = \frac{(qt)^n}{n!} e^{-qt}. \quad (6.1.25)$$

Proof of (6.1.24)

For the Poisson process (where events are independent), the probability of n events happening depends only on the time interval. Therefore we can write that the probability for one event happening in the time interval Δt is $P(n = 1, \Delta t) = P(1, \Delta t) = q\Delta t$. Based on that one gets

$$\begin{aligned} P(n, t + \Delta t) &= P(n, t; 0, \Delta t) + P(n-1, t; 1, \Delta t) \\ &= P(n, t)(1 - q\Delta t) + P(n-1, t)q\Delta t \\ P(n, t + \Delta t) - P(n, t) &= q\Delta t(P_{n-1} - P_n). \end{aligned}$$

Thus

$$\dot{p}_n = q(p_{n-1} - p_n).$$

Proof of (6.1.25)

We introduce the so-called generating function

$$G(s, t) = \sum_{n=0}^{\infty} s^n p_n(t)$$

where s is independent of time. Differentiating this function and substituting equation (6.1.12) in it gives

$$\begin{aligned}\frac{dG(s, t)}{dt} &= \sum_{n=0}^{\infty} s^n \dot{p}_n(t) \\ &= \sum_{n=0}^{\infty} s^n [q(p_{n-1} - p_n)] \\ &= qs \sum_{n=1}^{\infty} s^{n-1} p_{n-1}(t) - q \sum_{n=0}^{\infty} s^n p_n(t) \\ \frac{dG(s, t)}{dt} &= q(s-1)G(s, t) \\ G(s, t) &= G(s, 0) e^{q(s-1)t}.\end{aligned}$$

But, $G(s, 0) = \sum_{n=0}^{\infty} s^n p_n(0) = 1$ (only the $n = 0$ term survives, because one chooses the initial condition $p_n(0) = \delta_{n,0}$.) Thus

$$\begin{aligned}G(s, t) &= e^{q(s-1)t} = e^{qst} e^{-qt} \\ &= \sum_{n=0}^{\infty} \frac{(qst)^n}{n!} e^{-qt} \\ &= \sum_{n=0}^{\infty} s^n p_n(t)\end{aligned}$$

$$p_n(t) = \frac{(qt)^n}{n!} e^{-qt}.$$

An example of a linear one-step process is the decay process. Consider a piece of radioactive material. The number of active nuclei surviving at time $t > 0$, $N(t)$, is a non-stationary Markov process. To find the evolution of a collection of nuclei, let $P(n, t)$ be the probability that there are n surviving nuclei at time t .

If γ is the decay probability per unit time for one nucleus, the transition probability from n' to n in a short time Δt is (according to equation (6.1.8))

$$P_{1|1}(n, t + \Delta t | n', t) = \delta_{n',n} (1 - \gamma n' \Delta t) + \delta_{n'-1,n} \gamma n' \Delta t + \mathcal{O}(\Delta t)^2. \quad (6.1.26)$$

The second term is the decay probability for n' nuclei. In a very short time interval Δt one can expect not more than one of the n nuclei to decay. Hence the $\delta_{n'-1,n}$ in front of the decay probability. The first term corresponds to the case that no transition takes place. The transition probability can be written also as

$$P_{1|1}(n, t + \Delta t | n', t) = 0, n > n' \quad (6.1.27)$$

$$= n' \gamma \Delta t, n = n' - 1 \quad (6.1.28)$$

$$= \mathcal{O}(\Delta t)^2, n < n' - 1. \quad (6.1.29)$$

Therefore the transition probability per unit time is

$$W_{nn'} = \gamma n' \delta_{n,n'-1}. \quad (6.1.30)$$

Inserting this form in equation (6.1.12) gives the master equation for the decay process

$$\dot{p}_n(t) = \gamma(n+1)p_{n+1}(t) - \gamma np_n(t). \quad (6.1.31)$$

Now a device is applied for linear master equations which consist in multiplying both sides of equation (6.1.31) by n and summing over n . Relabeling indices n in the sum p_{n+1} , so to obtain p_n throughout one gets

$$\begin{aligned} \sum_{n=0}^{\infty} n\dot{p}_n &= \gamma \sum_{n=0}^{\infty} n(n+1)p_{n+1} - \gamma \sum_{n=0}^{\infty} n^2 p_n \\ &= \gamma \sum_{n=0}^{\infty} (n-1)np_n - \gamma \sum_{n=0}^{\infty} n^2 p_n \\ &= -\gamma \sum_{n=0}^{\infty} np_n. \end{aligned}$$

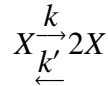
Thus the mean-field equation for $N(t)$ is given by

$$\frac{d}{dt} \langle N(t) \rangle = -\gamma \langle N(t) \rangle. \quad (6.1.32)$$

Solving the above equation for $\langle N(0) \rangle = n_0$, gives

$$\langle N(t) \rangle = n_0 e^{-\gamma t}. \quad (6.1.33)$$

An example of a nonlinear one-step process is a chemical reaction such as



k, k' are reaction coefficients, defined in chemical kinetics. For a state n , the generation probability per unit time g_n has the value kn . For the reverse reaction, one can assemble pairs of molecules of X , in $n(n-1)$ ways (this is a result of the combinations of n over 2, times 2, since each pair is counted twice). Thus $r_n = k'n(n-1)$.

Each reaction has a gain and a loss term. Therefore, in the master equation we will have two gain terms and two loss terms, thus four terms. For each reaction separately the gain and loss terms are as follows:

- $X_{(n)} \rightarrow 2X_{(n+1)}$: For this reaction, we are interested in the gain and loss of state X . Thus we call X state n , and $2X$ state $n+1$. Gain of X means destruction. Therefore the gain term for this reaction is $k'n(n+1)p_{n+1}$. Loss of X means generation. The loss term is then $-knp_n$.
- $X_{(n-1)} \leftarrow 2X_{(n)}$: For this reaction, one is interested in the gain and loss of state $2X$. Thus we call $2X$ state n , and X state $n-1$. Gain of $2X$ means generation. Therefore the gain term for this reaction is $k(n-1)p_{n+1}$. Loss of X means destruction. The loss term is then $-k'n(n-1)p_n$.

The master equation becomes

$$\dot{p}_n = k'n(n+1)p_{n+1} + k(n-1)p_{n-1} - knp_n - k'n(n-1)p_n. \quad (6.1.34)$$

Applying what was done in the linear case, one obtains

$$\begin{aligned}
\sum_{n=0}^{\infty} n \dot{p}_n &= k \sum_{n=0}^{\infty} n(n-1)p_{n-1} + k' \sum_{n=0}^{\infty} n^2(n+1)p_{n+1} - \\
&\quad \sum_{n=0}^{\infty} [k'n^2(n-1) + kn^2]p_n \\
&= k \sum_{n=0}^{\infty} n(n+1)p_n + k' \sum_{n=0}^{\infty} n(n-1)^2p_n - \\
&\quad \sum_{n=0}^{\infty} [k'n^2(n-1) + kn^2]p_n \\
&= k \sum_{n=0}^{\infty} np_n - k' \sum_{n=0}^{\infty} n(n-1)p_n.
\end{aligned}$$

This is not a closed equation due to the nonlinearity. So one needs a differential equation for $\langle n(n-1) \rangle$ and so on (infinite hierarchy). To simplify we make the mean-field approximation $\langle n(n-1) \rangle = \langle n \rangle \langle n \rangle$, so to obtain the mean-field equation for the chemical reaction

$$\frac{d}{dt} \langle n \rangle = k \langle n \rangle - k' \langle n \rangle^2. \quad (6.1.35)$$

6.2. Fractional Reaction-Diffusion

In view of the results

$$J_{-1/2}(x) = \sqrt{\frac{2}{\pi x}} \cos x. \quad (6.2.1)$$

and Mathai and Saxena (1978, p. 49), the cosine transform of the H-function is given by

$$\int_0^{\infty} t^{\rho-1} \cos(kt) H_{p,q}^{m,n} \left[at^{\mu} \left| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right. \right] dt \quad (6.2.2)$$

$$= \frac{\pi}{k^{\rho}} H_{q+1, p+2}^{n+1, m} \left[\frac{k^{\mu}}{a} \left| \begin{matrix} (1-b_q, B_q), (\frac{1+\rho}{2}, \frac{\mu}{2}) \\ (\rho, \mu), (1-a_p, a_p), (\frac{1+\rho}{2}, \frac{\mu}{2}) \end{matrix} \right. \right], \quad (6.2.3)$$

where $\Re[\rho + \mu_{1 \leq j \leq m}^{\min}(\frac{b_j}{B_j})] > 0$, $\Re[\rho + \mu_{1 \leq j \leq n}^{\max}(\frac{a_j-1}{A_j})] < 0$, $|\arg a| < \frac{1}{2}\pi$, $\Omega, \Omega > 0$; $k > 0$ and $\Omega = \sum_{j=1}^m B_j - \sum_{j=m+1}^q B_j + \sum_{j=1}^n a_j - \sum_{j=n+1}^p a_j$.

The Riemann-Liouville fractional integral of order ν is defined by

$${}_0D_t^{-\nu} N(x, t) = \frac{1}{\Gamma(\nu)} \int_0^t (t-u)^{\nu-1} N(x, u) du, \quad (6.2.4)$$

where $\Re(\nu) > 0$.

The following fractional derivative of order $\alpha > 0$ is introduced in the form

$$\begin{aligned} {}_0D_t^\alpha f(x, t) &= \frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{f^{(m)}(x, \tau) d\tau}{(t-\tau)^{\alpha+1-m}}, m-1 < \alpha \leq m, \Re(\alpha) > 0, m \in N. \\ &= \frac{\partial^m f(x, t)}{\partial t^m}, \text{ if } \alpha = m. \end{aligned} \quad (6.2.5)$$

where $\frac{\partial^m}{\partial t^m} f(x, t)$ is the m^{th} partial derivative of $f(x, t)$ with respect to t .

The Laplace transform of the Caputo derivative is given in the form

$$L\{{}_0D_t^\alpha f(x, t); s\} = s^\alpha F(x, s) - \sum_{r=0}^{m-1} s^{\alpha-r-1} f^{(r)}(x, 0+), \quad (m-1 < \alpha \leq m). \quad (6.2.6)$$

Following Feller, it is conventional to define the Riesz-Feller space-fractional derivative of order α and skewness θ in terms of its Fourier transform as

$$F\{{}_x D_\theta^\alpha f(x); k\} = -\Psi_\alpha^\theta(k) f^*(k), \quad (6.2.7)$$

where

$$\Psi_\alpha^\theta(k) = |k|^\alpha \exp[i(\text{sign}k)\frac{\theta\pi}{2}], \quad 0 < \alpha \leq 2, |\theta| \leq \min\{\alpha, 2-\alpha\}. \quad (6.2.8)$$

When $\theta = 0$, then (6.2.8) reduces to

$$F\{{}_x D_0^\alpha f(x); k\} = -|k|^\alpha, \quad (6.2.9)$$

which is the Fourier transform of the Weyl fractional operator, defined by

$${}_{-\infty}D_x^\mu f(t) = \frac{1}{\Gamma(n-\mu)} \frac{d^n}{dt^n} \int_{-\infty}^t \frac{f(u) du}{(t-u)^{\mu-n+1}}. \quad (6.2.10)$$

This shows that the Riesz-Feller operator may be regarded as a generalization of the Weyl operator.

Further, when $\theta = 0$, we have a symmetric operator with respect to x that can be interpreted as

$${}_x D_0^\alpha = -\left(-\frac{d^2}{dx^2}\right)^{\alpha/2}. \quad (6.2.11)$$

This can be formally deduced by writing $-(k)^\alpha = -(k^2)^{\alpha/2}$. For $0 < \alpha < 2$ and $|\theta| \leq \min\{\alpha, 2-\alpha\}$, the Riesz-Feller derivative can be shown to possess the following integral representation in the x domain:

$$\begin{aligned} {}_x D_\theta^\alpha f(x) &= \frac{\Gamma(1+\alpha)}{\pi} \left\{ \sin[(\alpha+\theta)\pi/2] \int_0^\infty \frac{f(x+\xi) - f(x)}{\xi^{1+\alpha}} d\xi \right. \\ &\quad \left. + \sin[(\alpha-\theta)\pi/2] \int_0^\infty \frac{f(x-\xi) - f(x)}{\xi^{1+\alpha}} d\xi \right\}. \end{aligned} \quad (6.2.12)$$

Finally, we need the following property of the H-function (Mathai and Saxena, 1978)

$$H_{p,q}^{m,n} \left[x^\delta \left| \begin{matrix} (a_p, a_p) \\ (b_q, B_q) \end{matrix} \right. \right] = \frac{1}{\delta} H_{p,q}^{m,n} \left[x \left| \begin{matrix} (a_p, A_p/\delta) \\ (b_q, B_q/\delta) \end{matrix} \right. \right], \quad (\delta > 0). \quad (6.2.13)$$

Unified Fractional Reaction-Diffusion Equation

In this section, we will investigate the solution of the reaction-diffusion equation (6.2.14) under the initial conditions (6.2.15). The result is given in the form of the following

Theorem 6.2.1. *Consider the unified fractional reaction-diffusion model*

$${}_0D_t^\beta N(x, t) = \eta_x D_\theta^\alpha N(x, t) + \Phi(x, t), \quad (6.2.14)$$

where $\eta, t > 0, x \in \mathbb{R}; \alpha, \theta, \beta$ are real parameters with the constraints $0 < \alpha \leq 2, |\theta| \leq \min(\alpha, 2 - \alpha), 0 < \beta \leq 2$, and the initial conditions

$$N(x, 0) = f(x), N_t(x, 0) = g(x); \text{ for } x \in \mathbb{R}, \lim_{|x| \rightarrow \infty} N(x, t) = 0, t > 0. \quad (6.2.15)$$

Here $N_t(x, 0)$ means the first partial derivative of $N(x, t)$ with respect to t evaluated at $t = 0$, η is a diffusion constant and $\Phi(x, t)$ is a nonlinear function belonging to the area of reaction-diffusion. Further ${}_x D_\theta^\alpha$ is the Riesz-Feller space-fractional derivative of order α and asymmetry θ . ${}_0D_t^\beta$ is the Caputo time-fractional derivative of order β . Then for the solution of (6.2.14), subject to the above constraints, there holds the formula

$$\begin{aligned} N(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f^*(k) E_{\beta, \alpha}(-\eta t^\beta \Psi_\alpha^\theta(k)) \exp(-ikx) dk \\ &+ \frac{1}{2\pi} \int_{-\infty}^{\infty} t g^*(k) E_{\beta, 2}(-\eta k^\alpha t^\beta \Psi_\alpha^\theta(k)) \exp(-ikx) dk \\ &+ \frac{1}{2\pi} \int_0^t \xi^{\beta-1} d\xi \int_{-\infty}^{\infty} \Phi^*(k, t - \xi) E_{\beta, \beta}(-\eta k^\alpha t^\beta \Psi_\alpha^\theta(k)) \exp(-ikx) dk. \end{aligned} \quad (6.2.16)$$

In equation (6.2.16) and the following, $E_{\alpha, \beta}(z)$ denotes the generalized Mittag-Leffler function.

Proof 6.2.1. If we apply the Laplace transform with respect to the time variable t , Fourier transform with respect to space variable x , and use the initial conditions (6.2.15) and the formula (6.2.7), then the given equation transforms into the form

$$s^\beta N^*(k, s) - s^{\beta-1} f^*(k) - s^{\beta-2} g^*(k) = -\eta \Psi_\alpha^\theta(k) N^*(k, s) + \Phi^*(k, s),$$

where according to the conventions followed, the symbol \sim will stand for the Laplace transform with respect to time variable t and $*$ represents the Fourier transform with respect to space variable x . Solving for N^* , it yields

$$N^*(k, s) = \frac{f^*(k) s^{\beta-1}}{s^\beta + \eta \Psi_\alpha^\theta(k)} + \frac{g^*(k) s^{\beta-2}}{s^\beta + \eta \Psi_\alpha^\theta(k)} + \frac{\Phi^*(k)}{s^\beta + \eta \Psi_\alpha^\theta(k)}. \quad (6.2.17)$$

On taking the inverse Laplace transform of (6.2.17) and applying the formula

$$L^{-1} \left\{ \frac{s^{\beta-1}}{a + s^\alpha} \right\} = t^{\alpha-\beta} E_{\alpha, \alpha-\beta+1}(-at^\alpha), \quad (6.2.18)$$

where $\Re(s) > 0$, $\Re(\alpha) > 0$, $\Re(\alpha - \beta) > -1$; it is seen that

$$\begin{aligned} N^*(k, t) &= f^*(k)E_{\beta,1}(-\eta t^\beta \Psi_\alpha^\theta(k)) + g^*(k)tE_{\beta,2}(-\eta t^\beta \Psi_\alpha^\theta(k)) \\ &+ \int_0^t \Phi^*(k, t - \xi) \xi^{\beta-1} E_{\beta,\beta}(-\eta \Psi_\alpha^\theta(k) \xi^\beta) d\xi. \end{aligned} \quad (6.2.19)$$

The required solution (6.2.16) is now obtained by taking the inverse Fourier transform of (6.2.19). This completes the proof of the theorem.

Special cases

When $g(x) = 0$, then by the application of the convolution theorem of the Fourier transform to the solution (6.2.16) of the theorem, it readily yields

Corollary 6.2.1. *The solution of the fractional reaction-diffusion equation*

$$\frac{\partial^\beta}{\partial t^\beta} N(x, t) - \eta \frac{\partial^\alpha}{\partial x^\alpha} N(x, t) = \Phi(x, t), \quad x \in R, t > 0, \eta > 0, \quad (6.2.20)$$

with initial conditions

$$N(x, 0) = f(x), N_t(x, 0) = 0 \text{ for } x \in R, 1 < \beta \leq 2, \lim_{x \rightarrow \pm\infty} N(x, t) = 0, \quad (6.2.21)$$

where η is a diffusion constant and $\Phi(x, t)$ is a nonlinear function belonging to the area of reaction-diffusion, is given by

$$\begin{aligned} N(x, t) &= \int_0^x G_1(x - \tau, t) f(\tau) d\tau \\ &+ \int_0^t (t - \xi)^{\beta-1} d\xi \int_0^x G_2(x - \tau, t - \xi) \Phi(\tau, \xi) d\tau, \end{aligned} \quad (6.2.22)$$

where

$$\begin{aligned} \rho &= \frac{\alpha - \theta}{2\alpha} \\ G_1(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-ikx) E_{\beta,1}(-\eta |t|^\beta |\Psi_\alpha^\theta(k)|) dk \\ &= \frac{1}{\alpha |x|} H_{3,3}^{2,1} \left[\frac{|x|}{\eta^{1/\alpha} t^{\beta/\alpha}} \left| \begin{matrix} (1,1/\alpha), (\beta, \beta/\alpha), (1, \rho) \\ (1,1), (1,1), (1, \rho) \end{matrix} \right. \right], \quad (\alpha > 0) \end{aligned} \quad (6.2.23)$$

and

$$\begin{aligned} G_2(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-ikx) E_{\beta,\beta}(-\eta |t|^\beta |\Psi_\alpha^\theta(k)|) dk \\ &= \frac{1}{\alpha |x|} H_{3,3}^{2,1} \left[\frac{|x|}{\eta^{1/\alpha} t^{\beta/\alpha}} \left| \begin{matrix} (1,1/\alpha), (\beta, \beta/\alpha), (1, \rho) \\ (1,1/\alpha), (1,1), (1, \rho) \end{matrix} \right. \right], \quad (\alpha > 0). \end{aligned} \quad (6.2.24)$$

In deriving the above results, we have used the inverse Fourier transform formula

$$F^{-1}[E_{\beta,\gamma}(-\eta t^\beta \Psi_\theta^\alpha(k)); x] = \frac{1}{\alpha|x|} H_{3,3}^{2,1} \left[\frac{|x|}{\eta^{1/\alpha} t^{\beta/\alpha}} \middle|_{(1,1/\alpha),(\gamma,\beta/\alpha),(1,\rho)}^{(1,1/\alpha),(1,1),(1,\rho)} \right], \quad (6.2.25)$$

where $\Re(\beta) > 0$, $\Re(\gamma) > 0$, which can be established by following a procedure.

Next, if we set $f(x) = \delta(x)$, $\Phi = 0$, $g(x) = 0$, where $\delta(x)$ is the Dirac delta-function, then we arrive at the following interesting result.

Corollary 6.2.2. Consider the following space-time fractional diffusion model

$$\frac{\partial^\beta N(x, t)}{\partial t^\beta} = \eta {}_x D_\theta^\alpha N(x, t), \quad \eta > 0, x \in R, \quad 0 < \beta \leq 2, \quad (6.2.26)$$

with the initial conditions $N(x, t = 0) = \delta(x)$, $N_t(x, 0) = 0$, $\lim_{x \rightarrow \pm\infty} N(x, t) = 0$ where η is a diffusion constant and $\delta(x)$ is the Dirac delta-function. Then for the fundamental solution of (6.2.26) with initial conditions, there holds the formula

$$N(x, t) = \frac{1}{\alpha|x|} H_{3,3}^{2,1} \left[\frac{|x|}{(\eta t^\beta)^{1/\alpha}} \middle|_{(1,1/\alpha),(1,1),(1,\rho)}^{(1,1/\alpha),(1,\beta/\alpha),(1,\rho)} \right], \quad (6.2.27)$$

where $\rho = \frac{\alpha-\theta}{2\alpha}$.

Some interesting special cases of (6.2.26) are enumerated below.

- (i) We note that for $\alpha = \beta$, the corresponding solution of (6.2.26), denoted by N_α^θ , which we call as the neutral fractional diffusion, can be expressed in terms of elementary function and can be defined for $x > 0$ as

Neutral fractional diffusion: $0 < \alpha = \beta < 2; \theta \leq \min\{\alpha, 2 - \alpha\}$,

$$N_\alpha^\theta(x) = \frac{1}{\pi} \frac{x^{\alpha-1} \sin[(\pi/2)(\alpha - \theta)]}{1 + 2x^\alpha \cos[(\pi/2)(\alpha - \theta)] + x^{2\alpha}}. \quad (6.2.28)$$

The neutral fractional diffusion is not studied at length in the literature.

Next we derive some stable densities in terms of the H-functions as special cases of the solution of the equation

- (ii) If we set $\beta = 1$, $0 < \alpha < 2; \theta \leq \min\{\alpha, 2 - \alpha\}$ then (6.2.26) reduces to space fractional diffusion equation, which we denote by $L_\alpha^\theta(x)$ is the fundamental solution of the following space-time fractional diffusion model:

$$\frac{\partial N(x, t)}{\partial t} = \eta {}_x D_\theta^\alpha N(x, t), \quad \eta > 0, x \in R, \quad (6.2.29)$$

with the initial conditions $N(x, t = 0) = \delta(x)$, $\lim_{x \rightarrow \pm\infty} N(x, t) = 0$, where η is a diffusion constant and $\delta(x)$ is the Dirac-delta function. Hence for the solution of (6.2.29) there holds the formula

$$L_\alpha^\theta(x) = \frac{1}{\alpha(\eta t)^{1/\alpha}} H_{2,2}^{1,1} \left[\frac{(\eta t)^{1/\alpha}}{|x|} \middle|_{(\frac{1}{\alpha}, \frac{1}{\alpha}), (\rho, \rho)}^{(1,1), (\rho, \rho)} \right], \quad 0 < \alpha < 1, |\theta| \leq \alpha, \quad (6.2.30)$$

where $\rho = \frac{\alpha - \theta}{2\alpha}$. The density represented by the above expression is known as α -stable Lévy density. Another form of this density is given by

$$L_\alpha^\theta(x) = \frac{1}{\alpha(\eta t)^{1/\alpha}} H_{2,2}^{1,1} \left[\frac{|x|}{(\eta t)^{1/\alpha}} \left| \begin{matrix} (1-\frac{1}{\alpha}, \frac{1}{\alpha}), (1-\rho, \rho) \\ (0,1), (1-\rho, \rho) \end{matrix} \right. \right], \quad 1 < \alpha < 2, |\theta| \leq 2 - \alpha, \quad (6.2.31)$$

- (iii) Next, if we take $\alpha = 2, 0 < \beta < 2, \theta = 0$, then we obtain the time fractional diffusion, which is governed by the following time fractional diffusion model:

$$\frac{\partial^\beta N(x, t)}{\partial t^\beta} = \eta \frac{\partial^2}{\partial x^2} N(x, t), \quad \eta > 0, x \in R, 0 < \beta \leq 2, \quad (6.2.32)$$

with the initial conditions $N(x, t = 0) = \delta(x), N_t(x, 0) = 0, \lim_{x \rightarrow \pm\infty} N(x, t) = 0$ where η is a diffusion constant and $\delta(x)$ is the Dirac delta-function, whose fundamental solution is given by the equation

$$N(x, t) = \frac{1}{2|x|} H_{1,1}^{1,0} \left[\frac{|x|}{(\eta t^\beta)^{1/2}} \left| \begin{matrix} (1, \beta/2) \\ (1,1) \end{matrix} \right. \right]. \quad (6.2.33)$$

- (iv) Further, if we set $\alpha = 2, \beta = 1$ and $\theta \rightarrow 0$ then for the fundamental solution of the standard diffusion equation

$$\frac{\partial}{\partial t} N(x, t) = \eta \frac{\partial^2}{\partial x^2} N(x, t), \quad (6.2.34)$$

with initial condition

$$N(x, t = 0) = \delta(x), \quad \lim_{x \rightarrow \pm\infty} N(x, t) = 0, \quad (6.2.35)$$

there holds the formula

$$N(x, t) = \frac{1}{2|x|} H_{1,1}^{1,0} \left[\frac{|x|}{\eta^{1/2} t^{1/2}} \left| \begin{matrix} (1, 1/2) \\ (1,1) \end{matrix} \right. \right] = (4\pi\eta t)^{-1/2} \exp\left[-\frac{|x|^2}{4\eta t}\right], \quad (6.2.36)$$

which is the classical Gaussian density.

Finally, for $\beta = 1/2$ in (6.2.14), we arrive at

Corollary 6.2.3. *Consider the following fractional reaction-diffusion model*

$$D_t^{1/2} N(x, t) = \eta_x D_\theta^\alpha N(x, t) + \Phi(x, t), \quad (6.2.37)$$

where $\eta, t > 0, x \in R; \alpha, \theta$ are real parameters with the constraints $0 < \alpha \leq 2, |\theta| \leq \min(\alpha, 2 - \alpha)$, and the initial conditions

$$N(x, 0) = f(x), \quad \text{for } x \in R, \quad \lim_{x \rightarrow \pm\infty} N(x, t) = 0. \quad (6.2.38)$$

Here η is a diffusion constant and $\Phi(x, t)$ is a nonlinear function belonging to the area of reaction-diffusion. Further ${}_x D_\theta^\alpha$ is the Riesz-Feller space fractional derivative of order α and asymmetry θ and $D_t^{1/2}$ is the Caputo time-fractional derivative of order $1/2$. Then for the solution of (6.2.37), subject to the above constraints, there holds the formula

$$\begin{aligned} N(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} f^*(k) E_{1/2,1}(-\eta t^\beta \Psi_\alpha^\theta(k)) \exp(-ikx) dk \\ &+ \frac{1}{2\pi} \int_0^t \xi^{-1/2} d\xi \int_{-\infty}^{\infty} \Phi^*(kct - \xi) E_{\frac{1}{2}, \frac{1}{2}}(-\eta k^\alpha t^{1.2} \Psi_\alpha^\theta(k)) \exp(-ikx) dk. \end{aligned} \quad (6.2.39)$$

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